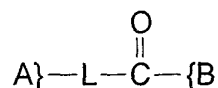


**WE CLAIM:**

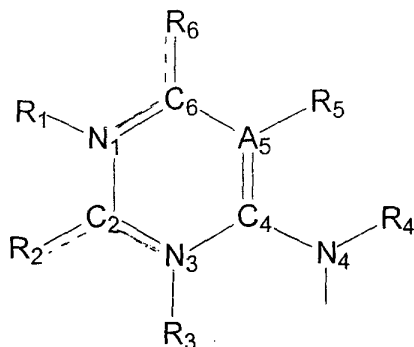
1. A pyrimidine derivative or analogue having the schematic structure:



where:

(a) A is an amino-substituted six-membered heterocyclic moiety of formula

(I)



where:

(i) if the bond between N<sub>1</sub> and C<sub>6</sub> is a single bond, then the bond between C<sub>6</sub> and R<sub>6</sub> is a double bond, R<sub>6</sub> is O or S, and R<sub>1</sub> is hydrogen, alkyl, aralkyl, cycloalkyl, or heteroaralkyl;

(ii) if the bond between N<sub>1</sub> and C<sub>6</sub> is a double bond, then the bond between C<sub>6</sub> and R<sub>6</sub> is a single bond, R<sub>1</sub> is not present, and R<sub>6</sub> is hydrogen, halo, amino, OQ<sub>1</sub>, SQ<sub>1</sub>, NHNH<sub>2</sub>, NHOQ<sub>1</sub>, NQ<sub>1</sub>Q<sub>2</sub>, or NHQ<sub>1</sub>, where Q<sub>1</sub> and Q<sub>2</sub> are alkyl, aralkyl, heteroaralkyl, aryl, heteroaryl, alkanoyl, aroyl, aralkanoyl, heteroaralkanoyl, heteroaroyl, alkylsulfonyl, arylsulfonyl, heteroarylsulfonyl, aralkylsulfonyl, or heteroaralkylsulfonyl in which the alkyl portions can be cyclic and can contain from 1 to 3 heteroatoms which can be N, O, or S, and when Q<sub>1</sub> and Q<sub>2</sub> are present together and are alkyl, they can be taken together to form a 5- or 6- membered ring which can contain 1 other heteroatom which can be N, O, or S, of which the N can be further substituted with Y<sub>2</sub>, where Y<sub>2</sub> is alkyl, aryl, heteroaryl, aralkyl, heteroaralkyl, alkanoyl,

aroyl, heteroaroyl, aralkanoyl, heteroaralkanoyl, alkylsulfonyl, arylsulfonyl, heteroarylsulfonyl, aralkylsulfonyl, heteroaralkylsulfonyl, alkoxycarbonyl, aryloxycarbonyl, heteroaryloxycarbonyl, aralkoxycarbonyl, heteroaralkoxycarbonyl, alkylaminocarbonyl, arylaminocarbonyl, heteroarylaminocarbonyl, aralkylaminocarbonyl, or heteroaralkylaminocarbonyl, in which the alkyl portions can be cyclic and can contain from 1 to 3 heteroatoms which can be N, O, or S;

(iii) if the bond between  $C_2$  and  $N_3$  is a single bond, then the bond between  $C_2$  and  $R_2$  is a double bond,  $R_2$  is O or S, and  $R_3$  is hydrogen or alkyl;

(iv) if the bond between  $C_2$  and  $N_3$  is a double bond, then the bond between  $C_2$  and  $R_2$  is a single bond,  $R_3$  is not present, and  $R_2$  is hydrogen, alkyl, aralkyl, cycloalkyl, heteroaralkyl, halo, amino,  $OQ_1$ ,  $SQ_1$ ,  $NHNH_2$ ,  $NHOQ_1$ ,  $NQ_1Q_2$ , or  $NHQ_1$ , where  $Q_1$  and  $Q_2$  are alkyl, aralkyl, heteroaralkyl, aryl, heteroaroyl, alkanoyl, aroyl, aralkanoyl, heteroaralkanoyl, heteroaroyl, alkylsulfonyl, arylsulfonyl, heteroarylsulfonyl, aralkylsulfonyl, or heteroaralkylsulfonyl in which the alkyl portions can be cyclic and can contain from 1 to 3 heteroatoms which can be N, O, or S, and when  $Q_1$  and  $Q_2$  are present together and are alkyl, they can be taken together to form a 5- or 6-membered ring which can contain 1 other heteroatom which can be N, O, or S, of which the N can be further substituted with  $Y_3$ , where  $Y_3$  is alkyl, aryl, heteroaroyl, aralkyl, heteroaralkyl, alkanoyl, aroyl, heteroaroyl, aralkanoyl, heteroaralkanoyl, alkylsulfonyl, arylsulfonyl, heteroarylsulfonyl, aralkylsulfonyl, heteroaralkylsulfonyl, alkoxycarbonyl, aryloxycarbonyl, heteroaryloxycarbonyl, aralkoxycarbonyl, heteroaralkoxycarbonyl, alkylaminocarbonyl, arylaminocarbonyl, heteroarylaminocarbonyl, aralkylaminocarbonyl, or heteroaralkylaminocarbonyl, in which the alkyl portions can be cyclic and can contain from 1 to 3 heteroatoms which can be N, O, or S;

(v)  $R_4$  is hydrogen, alkyl, aralkyl, heteroaralkyl, alkanoyl, aroyl, heteroaroyl, aralkanoyl, heteroaralkanoyl, alkylsulfonyl, arylsulfonyl, heteroarylsulfonyl, alkoxycarbonyl, aryloxycarbonyl, heteroaryloxycarbonyl, alkylaminocarbonyl, arylaminocarbonyl, or heteroarylaminocarbonyl;

(vi)  $A_5$  is carbon or nitrogen;

(vii) if  $A_5$  is nitrogen, then  $R_5$  is not present;

(viii) if  $A_5$  is carbon, then  $R_5$  is hydrogen, amino, alkyl, alkoxy, halo, nitro, aryl, cyano, alkenyl, or aralkyl;

(x) (ix)  $N_4$  is bonded to L;

(b) L is a hydrocarbonyl moiety of 1 to 6 carbon atoms that can be cyclic, with the hydrocarbonyl moiety being optionally substituted with one or more substituents selected from the group consisting of lower alkyl, amino, hydroxy, lower alkoxy, lower alkylamino, lower alkylthio and oxo; and

(c) B is -OZ or N( $Y_1$ )-D, where Z is hydrogen, alkyl, aryl, heteroaryl, cycloalkyl, aralkyl, or heteroaralkyl, D is a moiety that promotes absorption of the derivative or analogue, and  $Y_1$  is hydrogen, alkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl, which, when taken with D, can form a cyclic 5- or 6-membered saturated structure which can contain one other heteroatom which can be O, N, or S, of which N can be further substituted with  $Y_4$ , where  $Y_4$  is alkyl, aryl, heteroaryl, aralkyl, heteroaralkyl, alkanoyl, aroyl, heteroaroyl, aralkanoyl, heteroaralkanoyl, alkylsulfonyl, arylsulfonyl, heteroarylsulfonyl, aralkylsulfonyl, heteroaralkylsulfonyl, alkoxycarbonyl, aryloxycarbonyl, heteroaryloxycarbonyl, aralkoxycarbonyl, heteroaralkoxycarbonyl, alkylaminocarbonyl, arylaminocarbonyl, heteroarylaminocarbonyl, aralkylaminocarbonyl, or heteroaralkylaminocarbonyl, in which the alkyl portions can be cyclic and can contain from 1 to 3 heteroatoms which can be N, O, or S.

2. The pyrimidine derivative or analogue of claim 1 wherein  $A_5$  is carbon and the six-membered heterocyclic moiety is a pyrimidine moiety.

3. The pyrimidine derivative or analogue of claim 2 wherein  $R_2$  is O and  $R_3$  is hydrogen.

4. The pyrimidine derivative or analogue of claim 3 wherein R<sub>5</sub> is hydrogen, R<sub>6</sub> is amino, and the pyrimidine moiety is cytosine.
5. The pyrimidine derivative or analogue of claim 3 wherein R<sub>1</sub> is hydrogen, R<sub>5</sub> is methyl, R<sub>6</sub> is O, and the pyrimidine moiety is thymine.
6. The pyrimidine derivative or analogue of claim 3 wherein R<sub>1</sub> is methyl, R<sub>5</sub> is hydrogen, R<sub>6</sub> is O, and the pyrimidine moiety is uracil.
7. The pyrimidine derivative or analogue of claim 3 wherein R<sub>1</sub> is hydrogen, R<sub>5</sub> is methyl, R<sub>6</sub> is O, and the pyrimidine moiety is 3-methyluracil.
8. The pyrimidine derivative or analogue of claim 3 wherein R<sub>1</sub> is methyl, R<sub>5</sub> is methyl, R<sub>6</sub> is O, and the pyrimidine moiety is 3-methylthymine.
9. The pyrimidine derivative or analogue of claim 3 wherein R<sub>5</sub> is hydrogen, R<sub>6</sub> is methylamino, and the pyrimidine moiety is 4-methylcytosine.
10. The pyrimidine derivative or analogue of claim 3 wherein R<sub>5</sub> is methyl, R<sub>6</sub> is amino, and the pyrimidine moiety is 5-methylcytosine.
11. The pyrimidine derivative or analogue of claim 3 wherein R<sub>5</sub> is hydroxymethyl, R<sub>6</sub> is amino, and the pyrimidine moiety is 5-hydroxymethylcytosine.

12. The pyrimidine derivative or analogue of claim 3 wherein  $R_1$  is hydrogen,  $R_5$  is hydroxyl,  $R_6$  is O, and the pyrimidine moiety is 5-hydroxyuracil.
13. The pyrimidine derivative or analogue of claim 3 wherein  $R_1$  is hydrogen,  $R_5$  is carboxymethyl,  $R_6$  is O, and the pyrimidine moiety is 5-carboxymethyluracil.
14. The pyrimidine derivative or analogue of claim 3 wherein  $R_1$  is hydrogen,  $R_5$  is hydroxymethyl,  $R_6$  is O, and the pyrimidine moiety is 5-hydroxymethyluracil.
15. The pyrimidine derivative or analogue of claim 2 wherein  $R_2$  is S and  $R_3$  is hydrogen.
16. The pyrimidine derivative or analogue of claim 15 wherein  $R_1$  is hydrogen,  $R_5$  is hydrogen,  $R_6$  is O, and the pyrimidine moiety is 2-thiouracil.
17. The pyrimidine derivative or analogue of claim 15 wherein  $R_1$  is hydrogen,  $R_5$  is methylamino,  $R_6$  is O, and the pyrimidine moiety is 5-methylamino-2-thiouracil.
18. The pyrimidine derivative or analogue of claim 15 wherein  $R_1$  is hydrogen,  $R_5$  is methyl,  $R_6$  is O, and the pyrimidine moiety is 5-methyl-2-thiouracil.
19. The pyrimidine derivative or analogue of claim 15 wherein  $R_5$  is hydrogen,  $R_6$  is amino, and the pyrimidine derivative or analogue is 2-thiocytosine.
20. The pyrimidine derivative or analogue of claim 2 wherein  $R_2$  is amino and the bond between  $C_2$  and  $N_3$  is a double bond.

21. The pyrimidine derivative or analogue of claim 20 wherein  $R_1$  is hydrogen,  $R_5$  is hydrogen,  $R_6$  is O, and the pyrimidine moiety is 2-aminopyrimidinone.

22. The pyrimidine derivative or analogue of claim 20 wherein  $R_5$  is hydrogen,  $R_6$  is Cl, and the pyrimidine moiety is 2-amino-4-chloropyrimidine.

23. The pyrimidine derivative or analogue of claim 2 wherein  $R_2$  is hydrogen and the bond between  $C_2$  and  $N_3$  is a double bond.

24. The pyrimidine derivative or analogue of claim 23 wherein  $R_5$  is hydrogen,  $R_6$  is Cl, and the pyrimidine moiety is 4-chloropyrimidine.

25. The pyrimidine derivative or analogue of claim 23 wherein  $R_5$  is amino,  $R_6$  is Cl, and the pyrimidine moiety is 5-amino-4-chloropyrimidine.

26. The pyrimidine derivative or analogue of claim 23 wherein  $R_5$  is methyl,  $R_6$  is Cl, and the pyrimidine moiety is 4-chloro-5-methylpyrimidine.

27. The pyrimidine derivative or analogue of claim 23 wherein  $R_5$  is hydroxymethyl,  $R_6$  is Cl, and the pyrimidine moiety is 4-chloro-5-hydroxymethylpyrimidine.

28. The pyrimidine derivative or analogue of claim 23 wherein  $R_5$  is carboxymethyl,  $R_6$  is Cl, and the pyrimidine moiety is 4-chloro-5-carboxymethylpyrimidine.

29. The pyrimidine derivative or analogue of claim 23 wherein  $R_1$  is hydrogen, methyl, or ethyl,  $R_5$  is hydrogen, methyl, or ethyl, and  $R_6$  is O.

30. The pyrimidine derivative or analogue of claim 29 wherein  $R_1$  is hydrogen,  $R_5$  is hydrogen, and the pyrimidine moiety is pyrimidinone.

31. The pyrimidine derivative or analogue of claim 1 wherein L has the structure  $-(CH_2)_n-$  wherein n is an integer from 1 to 6.

32. The pyrimidine derivative or analogue of claim 31 wherein n is 2.

33. The pyrimidine derivative or analogue of claim 31 wherein n is 3.

34. The pyrimidine derivative or analogue of claim 1 wherein the moiety B is – OZ.

35. The pyrimidine derivative or analogue of claim 34 wherein Z is hydrogen.

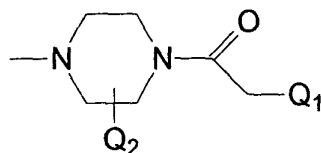
36. The pyrimidine derivative or analogue of claim 34 wherein Z is alkyl.

37. The pyrimidine derivative or analogue of claim 36 wherein Z is selected from the group consisting of methyl, ethyl, butyl, propyl, and isopropyl.

38. The pyrimidine derivative or analogue of claim 1 wherein the moiety B is N(Y<sub>1</sub>)-D.
39. The pyrimidine derivative or analogue of claim 38 wherein Y<sub>1</sub> is hydrogen.
40. The pyrimidine derivative or analogue of claim 38 wherein Y<sub>1</sub> is lower alkyl.
41. The pyrimidine derivative or analogue of claim 40 wherein Y<sub>1</sub> is methyl.
42. The pyrimidine derivative or analogue of claim 38 wherein D is a moiety having at least one polar, charged, or hydrogen-bond-forming group to increase the water-solubility of the pyrimidine derivative or analogue.
43. The pyrimidine derivative or analogue of claim 42 wherein D is a carboxylic acid or carboxylic acid ester with the structure
- $$\text{---}(\text{CH}_2)_p\text{---}\overset{\text{O}}{\underset{\parallel}{\text{C}}}\text{---OW}_1$$
- wherein p is an integer from 1 to 6 and W<sub>1</sub> is selected from the group consisting of hydrogen and lower alkyl.
44. The pyrimidine derivative or analogue of claim 43 wherein W<sub>1</sub> is hydrogen.
45. The pyrimidine derivative or analogue of claim 43 wherein W<sub>1</sub> is ethyl.

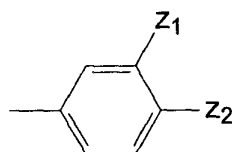


46. The pyrimidine derivative or analogue of claim 42 wherein D and Y<sub>1</sub> are taken together to form a piperazine derivative of the structure



wherein Q<sub>1</sub> is hydrogen, methyl, ethyl, butyl, or propyl, and Q<sub>2</sub> is hydrogen or methyl, where, if Q<sub>2</sub> is methyl, it can be located at either of the two possible positions in the piperazine ring.

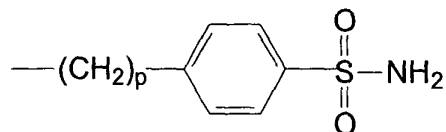
47. The pyrimidine derivative or analogue of claim 42 wherein D has the structure



where one of Z<sub>1</sub> and Z<sub>2</sub> is hydrogen, and the other of Z<sub>1</sub> and Z<sub>2</sub> is -COOH or -COOW<sub>1</sub>, wherein W<sub>1</sub> is alkyl.

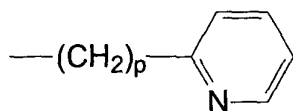
48. The pyrimidine derivative or analogue of claim 47 wherein W<sub>1</sub> is selected from the group consisting of methyl, ethyl, propyl, butyl, and isobutyl.

49. The pyrimidine derivative or analogue of claim 42 wherein D is a phenylsulfonamidyl moiety of the structure



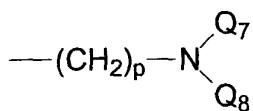
wherein p is an integer from 0 to 6.

50. The pyrimidine derivative or analogue of claim 42 wherein D is an alkylpyridyl moiety of structure



wherein p is an integer from 1 to 6.

51. The pyrimidine derivative or analogue of claim 42 wherein D is a dialkylaminoalkyl moiety of the structure



wherein p is an integer from 1 to 6 and Q<sub>7</sub> and Q<sub>8</sub> are alkyl, aralkyl, heteroaralkyl, aryl, heteroaryl, alkanoyl, aroyl, aralkanoyl, heteroaralkanoyl, or heteroaroyl in which the alkyl portions can be cyclic and can contain from 1 to 3 heteroatoms which can be N, O, or S, and when Q<sub>7</sub> and Q<sub>8</sub> are present together and are alkyl, they can be taken together to form a 5 or 6 member ring which may contain 1 other heteroatom which can be N, O, or S, of which the N may be further substituted with Y<sub>2</sub>, where Y<sub>2</sub> is alkyl, aryl, heteroaryl, aralkyl, heteroaralkyl, alkanoyl, aroyl, heteroaroyl, aralkanoyl, heteroaralkanoyl, alkylsulfonyl, arylsulfonyl, heteroarylsulfonyl, aralkylsulfonyl, heteroaralkylsulfonyl, alkoxycarbonyl, aryloxycarbonyl, heteroaryloxycarbonyl, aralkoxycarbonyl, heteroaralkoxycarbonyl, alkylaminocarbonyl, arylaminocarbonyl, heteroarylamino carbonyl, aralkylaminocarbonyl, or heteroaralkylaminocarbonyl, in which the alkyl portions can be cyclic and can contain from 1 to 3 heteroatoms which can be N, O, or S.

52. The pyrimidine derivative or analogue of claim 51 wherein Q<sub>7</sub> and Q<sub>8</sub> are each alkyl.

53. The pyrimidine derivative or analogue of claim 52 wherein  $Q_7$  and  $Q_8$  are each selected from the group consisting of methyl, ethyl, propyl, and isopropyl.

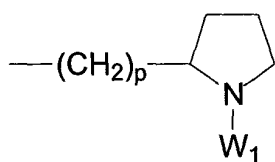
54. The pyrimidine derivative or analogue of claim 52 wherein  $Q_7$  and  $Q_8$  are taken together to form a five- or six-membered optionally substituted ring.

55. The pyrimidine derivative or analogue of claim 54 wherein the ring is a morpholinyl ring.

56. The pyrimidine derivative or analogue of claim 54 wherein the ring is a pyrrolidinyl ring that is optionally substituted with oxo.

57. The pyrimidine derivative or analogue of claim 54 wherein the ring is a piperidinyl ring that is optionally substituted with methyl or ethyl.

58. The pyrimidine derivative or analogue of claim 42 wherein D is an alkylpyrrolidinyl moiety of the structure



wherein  $p$  is an integer from 1 to 6 and  $W_1$  is selected from the group consisting of methyl, ethyl, and propyl.

59. The pyrimidine derivative or analogue of claim 1 that has a logP of from about 1 to about 4.

60. A pyrimidine derivative or analogue that is 4-[3-(2-amino-6-chloropyrimidin-4-ylamino)propionylamino] benzoic acid ethyl ester.

61. A pyrimidine derivative or analogue that is 4-[3-(6-chloropyrimidin-4-ylamino)propionylamino] benzoic acid ethyl ester.

62. A pyrimidine derivative or analogue that is 4-[3-(5-amino-6-chloropyrimidin-4-ylamino)propionylamino] benzoic acid ethyl ester.

63. A pyrimidine derivative or analogue that is 4-[3-(2-amino-6-chloropyrimidin-4-ylamino)propionylamino] benzoic acid.

64. A pyrimidine derivative or analogue that is 4-[3-(6-chloropyrimidin-4-ylamino)propionylamino] benzoic acid.

65. A pyrimidine derivative or analogue that is 4-[3-(5-amino-6-chloropyrimidin-4-ylamino)propionylamino] benzoic acid.

66. A pyrimidine derivative or analogue that is 3-[3-(2-amino-6-chloropyrimidin-4-ylamino)propionylamino] benzoic acid ethyl ester.

67. A pyrimidine derivative or analogue that is 3-[3-(6-chloropyrimidin-4-ylamino)propionylamino] benzoic acid ethyl ester.

68. A pyrimidine derivative or analogue that is 3-[3-(5-amino-6-chloropyrimidin-4-ylamino)propionylamino] benzoic acid ethyl ester.

69. A pyrimidine derivative or analogue that is 3-[3-(2-amino-6-chloropyrimidin-4-ylamino)propionylamino] benzoic acid.

70. A pyrimidine derivative or analogue that is 3-[3-(6-chloropyrimidin-4-ylamino)propionylamino] benzoic acid.

71. A pyrimidine derivative or analogue that is 3-[3-(5-amino-6-chloropyrimidin-4-ylamino)propionylamino] benzoic acid.